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Predictive theoretical simulations of materials properties: advances and challenges.

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Recent first-principles simulations of materials for fuel cells, hard coatings, piezoelectric sensors, and steels applications will be presented with the emphasis on the description of substitutional disorder problem. Examples of predictive power of the modern alloy theory will be given, but challenges will be discussed as well. In particular, we show how the doping of ceria is optimized from systematic first-principles simulations [1], followed by the experimental verification of the theoretical predictions. Theoretical description of the decomposition thermodynamics and mechanical properties of hard-coating (Ti-Al)N and (Cr-Al)N alloys will be presented, including the prediction of their behavior at high pressure [2]. The origin of the anomalous, 400% increase of the piezoelectric coefficient in $Sc_xAl_{1-x}N$ alloys will be revealed, and a strategy for a systematic search for new materials with high piezoelectric response will be outlined [3]. Finally, we discuss the magnetic structure of fcc Fe-Ni and Fe-Mn alloys [4], illustrating high demands on the accuracy of first-principles simulations.

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